Amendments to the Claims:

Please cancel claims 57, 106, 109, and 130-131, without prejudice or disclaimer, and amend claims 17, 33, 35, 46-54, 59-60, 63, 67-68, 70, 76, 78, 88, 90, 92, 102, 105, 108, 110, 120, 124, 129, and 132-138 as indicated in the following listing of claims, which replaces all prior versions and listings of claims in the application:

Listing of Claims:

1. (Original) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to tests of interactions between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target; and

a user interface allowing a user to view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

2. (Original) The computer system of claim 1, wherein the interaction includes binding and the effect includes inhibitory effect.

3. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity.

4. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds that have been or are being tested in preclinical studies in animals.

5. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds known to have an effect on the environment.

6. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include pharmacological reference agents.

7. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals in the market for clinical use for which there is a substantial amount of biological information available.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

8. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include drug candidates approved by the Food and Drug Administration for testing in humans.

9. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds obtained from natural sources that exhibit biological activity.

10. (Original) The computer system of claim 1, wherein the molecular targets include receptors.

11. (Withdrawn) The computer system of claim 1, wherein the molecular targets include enzymes.

12. (Withdrawn) The computer system of claim 1, wherein the molecular targets include nucleic acids.

13. (Withdrawn) The computer system of claim 1, wherein the molecular targets include carbohydrates.

14. (Original) The computer system of claim 1, wherein the records of the first database corresponding to a plurality of chemical compounds are organized in categories related to the description and properties of the compounds.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

15. (Original) The computer system of claim 14, wherein the categories include:

compound name;

compound type;

physical-chemical characteristics;

chemical space coordinates or structural descriptors; and

solubility.

16. (Original) The computer system of claim 1, wherein the first database includes a natural product database.

17. (Currently Amended) The computer system of claim 1, wherein the first database includes a ~~failed drug~~ database of chemical compounds that have failed in preclinical or human clinical tests.

18. (Original) The computer system of claim 1, wherein the first database includes a chemical registry database.

19. (Original) The computer system of claim 1, wherein the second database includes a three-dimensional structure database.

20. (Original) The computer system of claim 1, wherein the second database includes a sequence/mutation database.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

21. (Original) The computer system of claim 1, wherein the second database includes a genomic database.

22. (Original) The computer system of claim 1, wherein the records in the third database corresponding to biological information related to the chemical compounds effects on the biological targets, are organized in categories that include:

compound name;

target name;

toxicity;

side effects; and

mechanism of drug action.

23. (Original) The computer system of claim 1 further comprising means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold.

24. (Withdrawn) A method for analyzing data relevant to drug discovery and development comprising:

selecting chemical compounds from a first database containing records corresponding to a plurality of chemical compounds;

selecting molecular targets from a second database containing records corresponding to a plurality of molecular targets;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

producing information corresponding to the interactions between each of the selected chemical compounds and each of the selected molecular targets;

selecting a biological activity from a third database containing records corresponding to biological information related to effects of chemical compounds on biological targets; and

using the produced information to correlate patterns of interactions between chemical compounds and molecular targets associated with the selected biological activity.

25. (Withdrawn) The method of claim 24, wherein the step of producing information includes the steps of:

generating binding data of the binding between each of the selected chemical compounds and each of the selected molecular targets by monitoring the inhibitory effect that an unknown compound has on said binding;

setting a binding test threshold corresponding to the inhibitory effect; and

generating information on the combination of unknown compound, molecular target, and chemical compound that meets or fails to meet the binding test threshold.

26. (Withdrawn) The method of claim 25, wherein the binding data comprises positive and negative binding information.

27. (Previously Presented) The computer system of claim 1, wherein the interaction includes binding.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

28. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity or that have failed in preclinical or human clinical tests.

29. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds used in commerce as herbicides or pesticides.

30. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals approved for human clinical use by the Food and Drug Administration.

31. (Withdrawn) The computer system of claim 1, wherein the molecular targets include ion channels.

32. (Withdrawn) The computer system of claim 1, wherein the molecular targets include transporters or uptake sites.

33. (Currently Amended) A computer system comprising:

a first database ~~datastore~~ containing data corresponding to a plurality of chemical compounds;

a second database ~~datastore~~ containing data corresponding to a plurality of molecular targets;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a third database ~~datastore~~ containing data corresponding to tests of interactions between compounds in the first database ~~datastore~~ and molecular targets in the second database ~~datastore~~, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target; and

a user interface allowing a user to view information from the first database ~~datastore~~, the second database ~~datastore~~, and the third database ~~datastore~~ as it relates to a compound record in the first database ~~datastore~~ or as it relates to a molecular target in the second database ~~datastore~~ or as it relates to one or more interaction records in the third database ~~datastore~~.

34. (Previously Presented) The computer system of claim 33, wherein the chemical compounds include compounds with known biological activity.

35. (Currently Amended) A computer system comprising:

a first database containing data corresponding to a plurality of synthetic chemical compounds and data corresponding to biological information related to effects of such synthetic chemical compounds on biological systems;

a second database containing data corresponding to a plurality of molecular targets;

a third database containing data corresponding to tests of interactions between compounds in the first database and molecular targets in the second database; and

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

36. (Previously Presented) The computer system of claim 35, wherein the chemical compounds include compounds with known biological activity.

37. (Previously Presented) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets; and

a third database containing records corresponding to tests of interactions between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target.

38. (Previously Presented) The computer system of claim 37, further comprising:

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to a compound record in the first database.

39. (Previously Presented) The computer system of claim 37, further comprising:

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to a molecular target in the second database.

40. (Previously Presented) The computer system of claim 37, further comprising:

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to one or more interaction records in the third database.

41. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding.

42. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding and the effect includes inhibitory effect.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

43. (Previously Presented) The computer system of claim 37, wherein the chemical compounds include compounds with known biological activity.

44. (Withdrawn) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining (i) a first set of information associated with one or more chemical compounds, (ii) a second set of information associated with one or more molecular targets, and (iii) a third set of information reflecting an interaction between the chemical compounds and the molecular targets, wherein the process may provide, based on one or more queries, information reflecting a relationship between a chemical compound included in the first set, a molecular target included in the second set, and the information included in the third set.

45. (Withdrawn) In a system for correlating data associated with chemical compounds and molecular targets, a memory comprising:

a first array of records, each including information indicative of a chemical compound;

a second array of records, each including information indicative of a molecular target;

a third array of records, each corresponding to a binding capability between each of the chemical compounds and molecular targets; and

a fourth array of records, each corresponding to a biological activity related to the chemical compounds and the molecular targets,

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

wherein a process may access the first, second, and third arrays to produce information corresponding to a drug potential for a new compound based on relationships between characteristics associated with the new compound and a selected biological activity included in the fourth array of records or patterns of binding capabilities included in the third array.

46. (Currently Amended) A database ~~memory device~~ for storing data for access by a process executed by a processor, the database ~~memory device~~ comprising:

a compound data structure including data associated with a set of synthetic chemical compounds;

a target data structure including data associated with a set of molecular targets; and

a result data structure including data corresponding to results of screening tests between chemical compounds and molecular targets,

wherein the process determines a relationship between the data included in the compound, target, and result data structures.

47. (Currently Amended) The database ~~memory device~~ of claim 46, wherein the results include information on an effect a selected compound has on a known interaction of another compound with a selected molecular target and an effect of the selected compound with the selected molecular target.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

48. (Currently Amended) The database ~~memory device~~ of claim 46, wherein the synthetic chemical compounds include at least one of:

(i) compounds with known biological activity,

(ii) compounds tested in animals,

(iii) compounds known to have an effect on the environment,

(iv) pharmacological reference agents,

(v) known pharmaceuticals that have available preexisting biological information, and

(vi) compounds approved by a government agency for testing in humans~~, and~~

~~(vii) compounds obtained from natural sources that exhibit biological activity~~.

49. (Currently Amended) The database ~~memory device~~ of claim 46, wherein the molecular targets include at least one of:

(i) receptors,

(ii) enzymes,

(iii) nucleic acids,

(iv) carbohydrates,

(v) ion channels, and

(vi) transporters or uptake sites.

50. (Currently Amended) The database ~~memory device~~ of claim 46, wherein the process also provides a graphical interface including a description and properties of a selected chemical compound included in the compound data structure.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

51. (Currently Amended) The database ~~memory device~~ of claim 50, wherein the graphical interface includes a representation of at least one of the selected compound's name, type, structure, physical-chemical characteristics, chemical structural descriptors, and solubility.

52. (Currently Amended) The database ~~memory device~~ of claim 46, including a biological data structure including information corresponding to biological information related to an effect of each chemical compound included in the compound data structure on each molecular target included in the target data structure.

53. (Currently Amended) The database ~~memory device~~ of claim 52, wherein the biological information includes at least one of side effects, toxicity, and mechanism of drug action.

54. (Currently Amended) In a system for maintaining test screening results, a storage device for storing data for access by a process being executed by a processor comprising:

a data set including information corresponding to results of tests that show an interaction between selected chemical compounds and selected molecular targets, the tests including information on the effect that a compound from the selected chemical compounds has on the interaction of a compound known to interact with a molecular target from the selected molecular targets and said molecular target,

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

wherein the process provides selected result information to another data set based on a request associated with a selected chemical compound or molecular target.

55. (Previously Presented) The system of claim 54, wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

56. (Previously Presented) The system of claim 54, wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

57. (Canceled)

58. (Withdrawn) A system comprising:

a memory including one or more data arrays of information associated with chemical compounds and molecular targets; and

a processor for executing a process for providing a user interface including:

a representation of a selected chemical compound,

description information associated with the selected chemical compound, and

biological information associated with the selected chemical compound.

59. (Currently Amended) A computer system comprising:

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a first database containing records corresponding to a plurality of ~~known biologically active~~ synthetic chemical compounds,

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

60. (Currently Amended) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between all ~~or substantially all~~ of the compounds selected to comprise a compound set in the first database and all or substantially all of the molecular targets selected to comprise a molecular target set in the second database.

61. (Previously Presented) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

62. (Previously Presented) The computer system of claim 59, further comprising:

a fourth database containing records corresponding to the effect of chemical compounds contained in the first database on biological systems

63. (Currently Amended) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between all ~~or substantially all~~ of the compounds selected to comprise a compound set in the first database and all or substantially all of the molecular targets selected to comprise a molecular target set in the second database.

64. (Previously Presented) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

65. (Withdrawn) The computer system of claim 59, wherein the first database contains records corresponding to a plurality of known biologically active chemical compounds selected from among representatives of the following categories:

(a) pharmacological reference agents used in receptor, ion channel, transporter, or enzyme screening assays;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

(b) drug candidates that have been approved by the Food and Drug Administration for testing in humans, including those that have been discontinued from further development; and

(c) pharmaceuticals that have been approved for human clinical use by the Food and Drug Administration, including those that have been subsequently withdrawn from the market.

66. (Withdrawn) The computer system of claim 65, wherein the known biologically active compounds included in the first database are further selected from among the following:

compounds that have been tested in preclinical studies in animals;

pesticides;

herbicides;

bioactive natural products;

agricultural chemicals; and

environmental chemicals.

67. (Currently Amended) The computer system of claim 59, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters ~~or uptake sites~~; and

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

(d) enzymes.

68. (Currently Amended) The computer system of claim 65, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters ~~or uptake sites~~; and

(d) enzymes.

69. (Withdrawn) The computer system of claim 67, wherein the molecular targets in the second database are related to drug discovery and development.

70. (Currently Amended) The computer system of claim 59, wherein the third database contains records corresponding to ~~statistically~~ complete sets of results from a screening process ~~of tests to determine the interaction between compounds in the first database and targets in the second database~~.

71. (Previously Presented) The computer system of claim 59, wherein the records in the third database corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database includes positive interactions and negative or lack of interactions.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

72. (Previously Presented) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database are based on binding interactions.

73. (Previously Presented) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure the inhibition of binding by a compound in the first database with respect to a target in the second database in the presence of another compound, such as a reference agent or enzyme substrate, known to interact with the target.

74. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database are ligand binding assays.

75. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database are enzyme inhibition assays.

76. (Currently Amended) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure functional activity ~~activation, functional enhancement, functional inhibition, or lack of functional effect with respect to the molecular target~~.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

77. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database measure adenyl cyclase activity, inositol triphosphate, or neurotransmitter transport.

78. (Currently Amended) The computer system of claim 59, wherein the tests used to generate results comprising the third database are based on reporter gene assays or ~~cellular~~ functional assays.

79. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as numerical values.

80. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as per cent inhibition values.

81. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as potency values.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

82. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values exceed a specified threshold.

83. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall below a specified threshold.

84. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall between specified upper and lower thresholds.

85. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

86. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or of meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database and in formats that allow comparisons to be made (a) between such profiles among subsets of compounds in the first database or (b) between such profiles or groups of profiles of compounds in the first database and a comparable profile of interaction data for a compound or group of compounds not in the first database.

87. (Previously Presented) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set comprising LOPAC (List Of Pharmacologically Active Compounds, Sigma/RBI).

88. (Currently Amended) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set contained in ~~the~~ United States Pharmacopeial Convention Inc.'s USP DI Series ~~U.S. Pharmacopeia Drug Information for the Health Care Professional (USP DI) publication~~.

89. (Currently Amended) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include at least one of the following:

chemical name;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

chemical formula;

chemical structure;

molecular weight;

physical chemical properties;

chemical space coordinates;

chemical structural descriptors;

solubility; and

logP.[[.]]

90. (Currently Amended) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that ~~are organized in a format amenable to~~ can be searched and analyzed using computer-based searching and data analysis methods.

91. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database are organized by chemical structural relatedness or as chemical descriptor arrays or tables.

92. (Currently Amended) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that ~~are organized in a format amenable to data analysis~~ can be analyzed using methods of recursive partitioning.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

93. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using CoMFA software or related methods.

94. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using Catalyst/Hypo software or related methods.

95. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include SMILES codes.

96. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 2-D topological descriptors.

97. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 3-D pharmacophore descriptors.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

98. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include substructure or chemical moiety descriptors.

99. (Previously Presented) The computer system of claim 59, wherein the first database also contains records corresponding to biological information related to effects of the chemical compounds on biological systems.

100. (Previously Presented) The computer system of claim 99, wherein the records in the first database corresponding to biological information includes information on chemical name, trade names, or alternative compound names and at least one of the following categories:

toxicity;

side effects;

mechanism of action; and

pharmacokinetics.

101. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to pharmacokinetic effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

bioavailability;

absorption;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

drug distribution;

drug metabolism;

drug excretion;

blood-protein binding; and

blood-brain barrier passage.

102. (Currently Amended) The computer system of claim 100, wherein records in the first database corresponding to biological information related to toxicological effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

teratotoxicity;

mutagenicity; and

toxicity

~~hepatotoxicity;~~

~~renal toxicity;~~

~~neurotoxicity; and~~

~~cardiotoxicity~~.

103. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to side effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

known receptor interactions;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

known enzyme interactions;

behavioral effect;

physiological effect; and

organ effects.

104. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to mechanism of action of selected chemical compounds on biological systems includes information on at least one of the following categories:

target organ;

major pathway;

minor pathway; and

putative molecular target for mode of action.

105. (Currently Amended) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems ~~are organized in a format amenable to~~ can be searched and analyzed using computer-based searching and data analysis methods.

106. (Canceled)

107. (Previously Presented) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

biological systems are encoded using numerical terms such as LD50, ED50, percent absorbed, half-life, and peak concentration.

108. (Currently Amended) The computer system of claim 59, wherein the targets in the second database are selected from among those comprising the superfamily of G-Protein Coupled Receptors, including the following types and subtypes: dopamine, serotonin, adrenergic, muscarinic/acetylcholine, histamine, adenosine, angiotensin, bradykinin, C5a, chemokine, CCK, endothelin, neuropeptide Y, neurotensin, opioid, somatostatin, tachykinin, vasopressin, galanin, prostanoid, ~~purinoceptors,~~ cannabinoid, platelet-activating factor, thyrotropin releasing factor, leukotriene, corticotropin releasing factor, PACAP, vasoactive intestinal peptide, melatonin, glutamate, and GABA-B.

109. (Canceled)

110. (Currently Amended) The computer system of claim 59, wherein the targets in the second database are selected from among those ~~comprising nuclear receptors~~ non-steroidal or steroidal intracellular receptors, including estrogen, glucocorticoid, progesterone, and testosterone ~~androgen~~.

111. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise kinases or phosphatases.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

112. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising cytochrome P450 enzymes.

113. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising DNA-modifying enzymes or transferases.

114. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising neurotransmitter-related enzymes.

115. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise proteases or carbohydrates.

116. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include nucleic acids.

117. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include carbohydrates.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

118. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among sodium, potassium, calcium, chloride, or ligand-gated channels.

119. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among transporters or uptake sites for dopamine, serotonin, norepinephrine, adenosine, glycine, glutamate, and choline.

120. (Currently Amended) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database include at least one of the following:

molecular target name;

molecular target family, classification or type;

corresponding gene DNA sequence;

amino acid sequence;

3-dimensional conformation or structure;

~~differential expression across different cell types~~

location of expression in tissues or cell types;

hydropathy plots; and

biochemical or molecular descriptors.

121. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized in a format amenable to computer-based searching and data analysis methods.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

122. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence alignments.

123. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence homology.

124. (Currently Amended) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are grouped by family, superfamily, or subfamily ~~organized according to phylogenetic trees~~.

125. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by species source of the molecular target used in the test to determine the interaction between chemicals and targets.

126. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by location of expression in tissues.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

127. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by major or minor pathways.

128. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of molecular target protein expression across different cell types.

129. (Currently Amended) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of ~~molecular target messenger RNA expression~~ location of expression or across different cell types.

130. (Canceled)

131. (Canceled)

132. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of synthetic chemical compounds,

a second database containing records corresponding to a plurality of molecular targets;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a third database containing records corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

133. (Currently Amended) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining information identifying a plurality of chemical compounds and a plurality of molecular targets, wherein the data structure further maintains a set of information corresponding to results of tests to determine the interaction between the plurality of chemical compounds and the plurality of molecular targets, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

134. (Currently Amended) The memory of claim 133 [[134]], wherein the chemical compounds are known biologically active chemical compounds.

135. (Currently Amended) The memory of claim 133 [[134]], wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

136. (Currently Amended) The memory of claim 133 [[134]], wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

137. (Currently Amended) The memory of claim 133 [[134]], wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between all or substantially all of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and all or substantially all of a plurality of molecular targets selected to comprise a molecular target set in a molecular target data structure.

138. (Currently Amended) The memory of claim 133 [[134]], wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between a majority of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and a majority of a plurality of

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

molecular targets selected to comprise a molecular target set in a molecular target data structure.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com